ENABLING COMPUTATIONAL DYNAMICS IN DISTRIBUTED COMPUTING ENVIRONMENTS USING A HETEROGENEOUS COMPUTING TEMPLATE

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GOAL OF OUR WORK…

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MODELING AND SIMULATION, TESTING AND VALIDATION

- Use High Performance Computing (HPC) to simulate the dynamics of real-life engineering mechanical systems at unprecedented levels of accuracy

- HPC hardware targeted:
  - Cluster of CPUs and GPUs (accelerators)
    - More than 100 CPU cores, tens of GPU cards, tens of thousands of GPU cores

Talk Overview

- Overview of the engineering problems of interest
- Large-scale Multibody Dynamics
  - Problem formulation, solution method, and parallel implementation
- Overview of Heterogeneous Computing Template (HCT)
- Numerical Experiments
- Conclusions

Computational Multibody Dynamics

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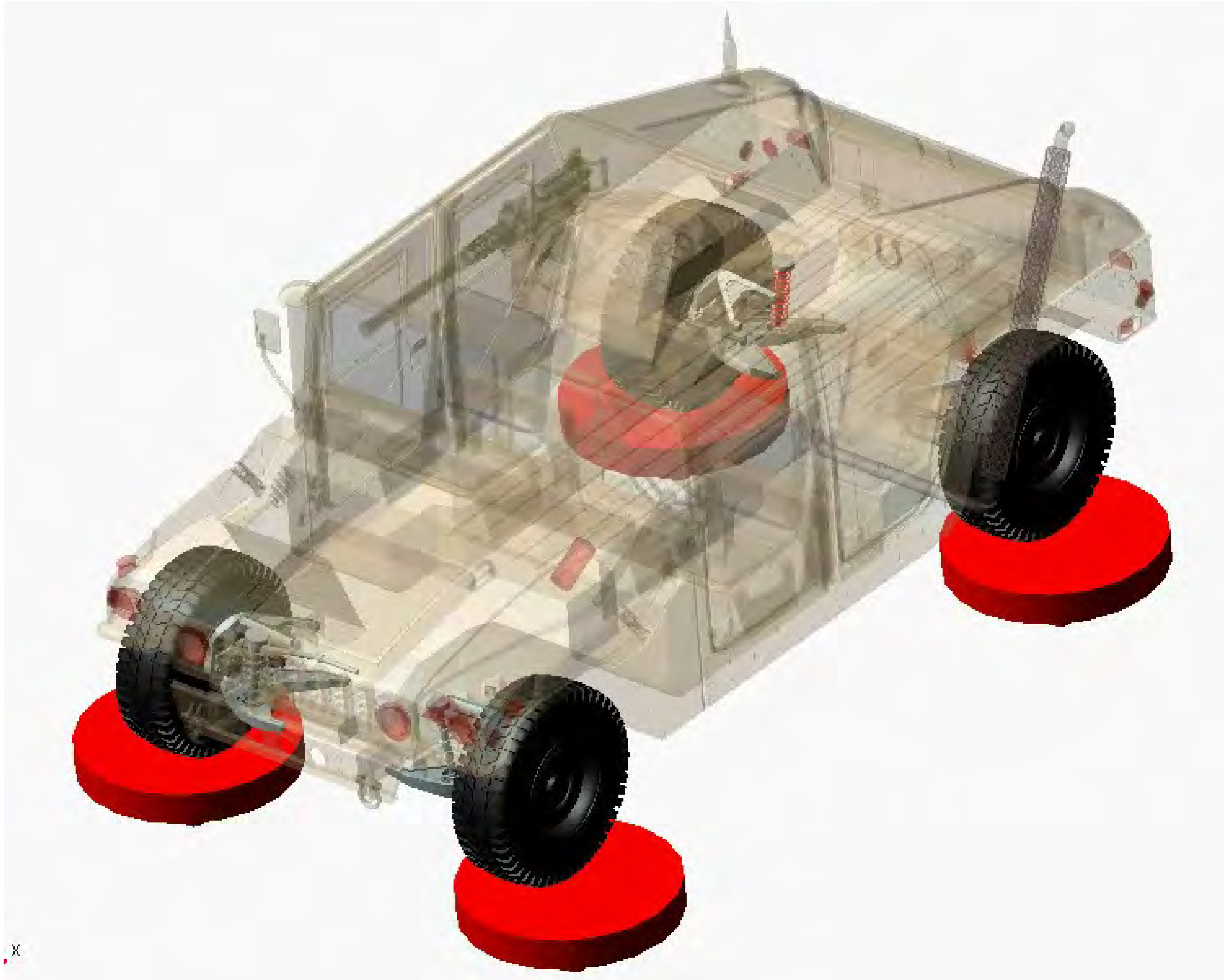
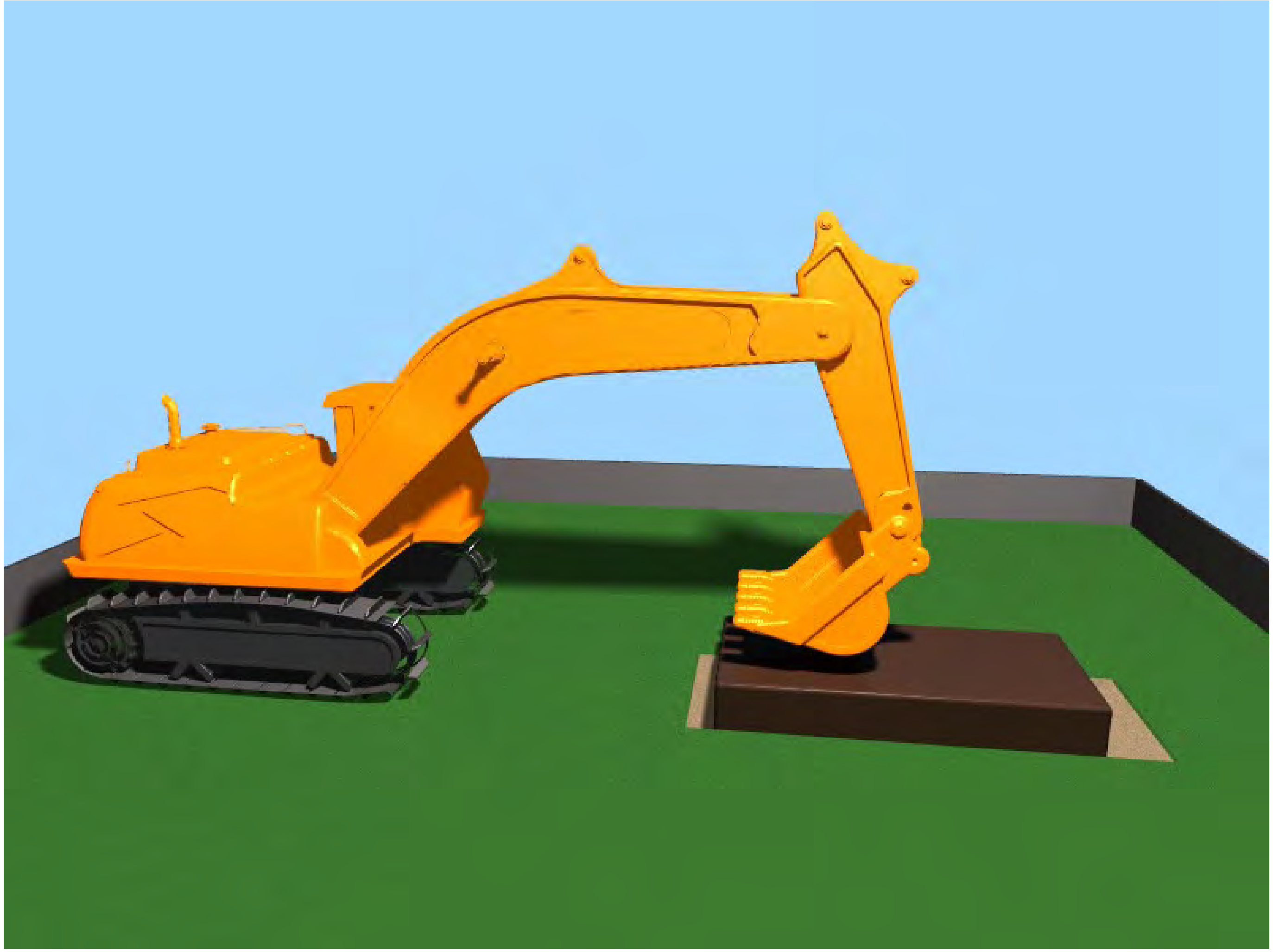
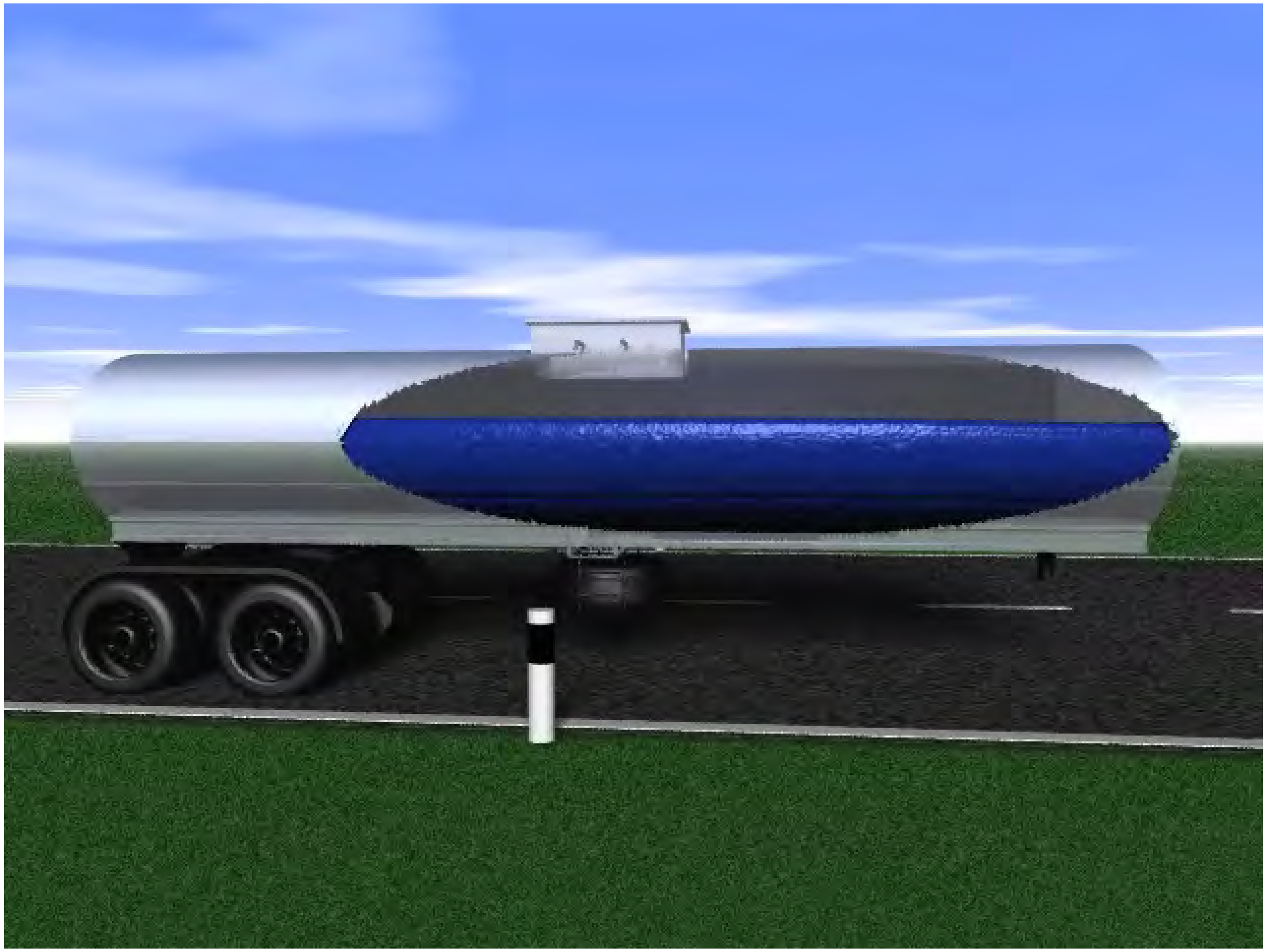


Multi-Physics…

Fluid-Solid Interaction: Navier-Stokes + Newton-Euler.



Computational Dynamics

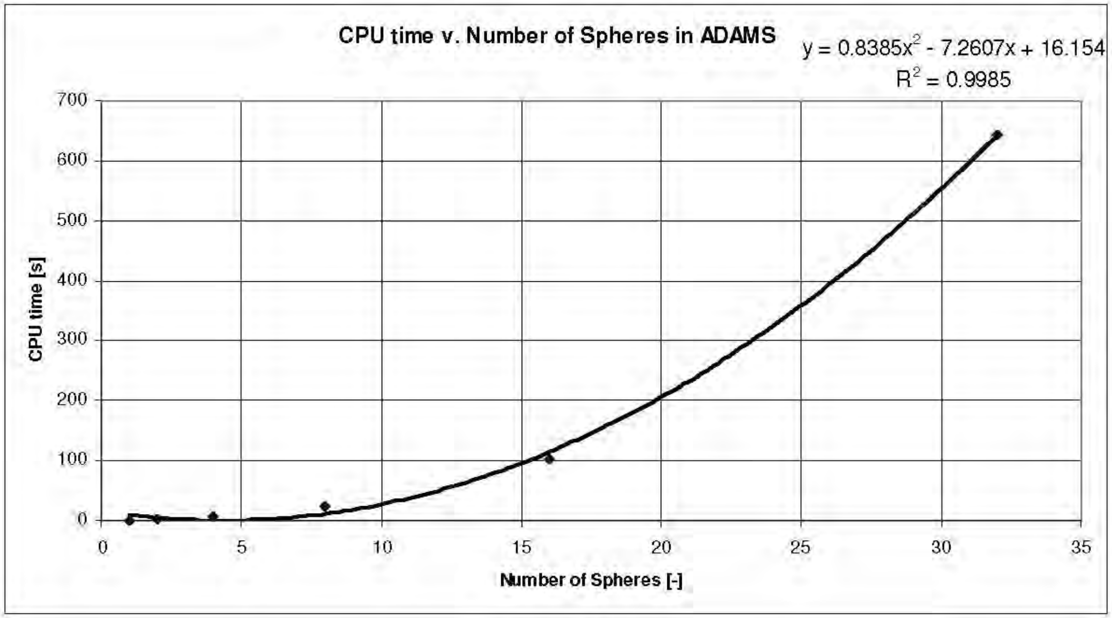


Rover Mobility on Granular Terrain

- Wheeled/tracked vehicle mobility on granular terrain
- Also interested in scooping and loading granular material

Frictional Contact Simulation
[Commercial Solution]

- Model Parameters:
  - Spheres: 60 mm diameter and mass 0.882 kg
  - Forces: smoothing with stiffness of 1E5, force exponent of 2.2, damping coefficient of 10.0, and a penetration depth of 0.1
  - Simulation length: 3 seconds



Frictional Contact: Two Different Approaches

- Discrete Element Method (DEM) - draws on a “smoothing” (penalty) approach
  - Lots of heuristics
  - Slow
  - General purpose
  - Used in ADAMS
- DVI-based (Differential Variational Inequalities)
  - A set of differential equations combined with inequality constraints
  - Fast (stable for significantly larger integration step-sizes)
  - Less general purpose
  - Used widely in computer games

The Modeling Component

Equations of Motion
Multibody Dynamics

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Generalized Positions

Generalized Mass Matrix

Velocity Transformation Matrix

Generalized Velocities

Kinematic Differential Equations →

$$\dot{\mathbf{q}} = \mathbf{T}(\mathbf{q})\mathbf{v}$$

Force Balance Equations →

$$\mathbf{M}(\mathbf{q})\dot{\mathbf{v}} = \underbrace{\mathbf{f}(t,\mathbf{q},\mathbf{v})}_{\text{Applied Force}} - \overbrace{\mathbf{g}_{\mathbf{q}}^{\mathrm{T}}(\mathbf{q},t)\boldsymbol{\lambda}}^{\text{Reaction Force}} + \overbrace{\sum_{i=1}^{N_c}(\gamma_n^i \mathbf{D}_n^{T,i} + \gamma_u^i \mathbf{D}_u^{T,i} + \gamma_w^i \mathbf{D}_w^{T,i})}^{\text{Frictional Contact Force}}$$

Holonomic Kinematic Constraints →

$$\mathbf{g}(\mathbf{q},t) = \mathbf{0}$$

Contact Complementarity Conditions →

$$0 \le \Phi^i(\mathbf{q},t) \perp \overbrace{\gamma_n^i}^{\text{Contact Impulse, for Contact "}i\text{"}} \ge 0 \qquad i = 1,2,\ldots,\underbrace{N_c}_{\text{Total Number of Contacts}}$$

Coulomb Friction Model →

$$(\gamma_u^i, \gamma_w^i) = \operatorname*{arg\,min}_{\mu^i \gamma_n^i \ge \sqrt{(\gamma_u^i)^2 + (\gamma_w^i)^2}} \underbrace{(\gamma_u^i \mathbf{v}^T \mathbf{D}_u^i + \gamma_w^i \mathbf{v}^T \mathbf{D}_w^i)}_{\text{Friction Dissipation Energy}}$$

Gap Function, for Contact "*i*"

Friction Impulse Components, for Contact "*i*"

Traditional Discretization Scheme

positions

time step index

$$\boxed{\mathbf{q}}^{(l+1)} = \mathbf{q}^{\boxed{(l)}} + h\mathbf{L}(\mathbf{q}^{(l)})\mathbf{v}^{(l+1)}$$

Mass Mat.

speeds

Applied Forces

Reaction impulses

$$\boxed{\mathbf{M}}(\mathbf{v}^{(l+1)} - \boxed{\mathbf{v}^{l}}) = h\mathbf{f}(t^{(l)}, \mathbf{q}^{(l)}, \mathbf{v}^{(l)}) + \sum_{i \in \mathcal{A}(q^{(l)},\delta)} \left(\boxed{\gamma_{i,n}\,\mathbf{D}_{i,n}} + \boxed{\gamma_{i,u}\,\mathbf{D}_{i,u}} + \boxed{\gamma_{i,w}\,\mathbf{D}_{i,w}}\right)$$

$$i \in \mathcal{A}(q^{(l)}, \delta): \quad 0 \leq \boxed{\frac{1}{h}\Phi_i(\mathbf{q}^{(l)})} + \mathbf{D}_{i,n}^T \mathbf{v}^{(l+1)} \boxed{\perp} \gamma_n^i \geq 0,$$

Complementarity Condition

$$(\gamma_{i,u}, \gamma_{i,w}) = \underset{\mu_i \gamma_{i,n} \geq \sqrt{\gamma_{i,u}^2 + \gamma_{i,w}^2}}{\operatorname{argmin}} \quad \mathbf{v}^T\left(\gamma_{i,u}\,\mathbf{D}_{i,u} + \gamma_{i,w}\,\mathbf{D}_{i,w}\right).$$

Stabilization term

Coulomb 3D fricion model

(Stewart & Trinkle, 1996)

Relaxed Discretization Scheme

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$$
\begin{aligned}
\mathbf{q}^{(l+1)} &= \mathbf{q}^{(l)} + h\mathbf{L}(\mathbf{q}^{(l)})\mathbf{v}^{(l+1)} \\
\mathbf{M}(\mathbf{v}^{(l+1)} - \mathbf{v}^{l}) &= h\mathbf{f}(t^{(l)}, \mathbf{q}^{(l)}, \mathbf{v}^{(l)}) + \textstyle\sum_{i \in \mathcal{A}(q^{(l)},\delta)} \left(\gamma_{i,n}\,\mathbf{D}_{i,n} + \gamma_{i,u}\,\mathbf{D}_{i,u} + \gamma_{i,w}\,\mathbf{D}_{i,w}\right) \\
i \in \mathcal{A}(q^{(l)},\delta):\quad 0 &\leq \tfrac{1}{h}\Phi_i(\mathbf{q}^{(l)}) + \mathbf{D}_{i,n}^{T}\mathbf{v}^{(l+1)} - \underbrace{\boxed{\mu^i\sqrt{(\mathbf{v}^T\,\mathbf{D}_{i,u})^2 + \mathbf{v}^T\,\mathbf{D}_{i,w})^2}}}_{\text{Relaxation Term}} \perp \gamma_n^i \geq 0, \\
(\gamma_{i,u}, \gamma_{i,w}) &= \underset{\mu_i\gamma_{i,n} \geq \sqrt{\gamma_{i,u}^2 + \gamma_{i,w}^2}}{\operatorname{argmin}} \quad \mathbf{v}^T\left(\gamma_{i,u}\,\mathbf{D}_{i,u} + \gamma_{i,w}\,\mathbf{D}_{i,w}\right).
\end{aligned}
$$

(Anitescu & Tasora, 2008)

The Cone Complementarity Problem [CCP]

- Overall approach assume the form of a Cone Complementarity Problem (CCP)

- Introduce the convex hypercone...

$$\Upsilon = \left(\bigoplus_{i \in \mathcal{A}(\mathbf{q}^l, \epsilon)} \mathcal{FC}^i \right)$$

... and its polar hypercone:

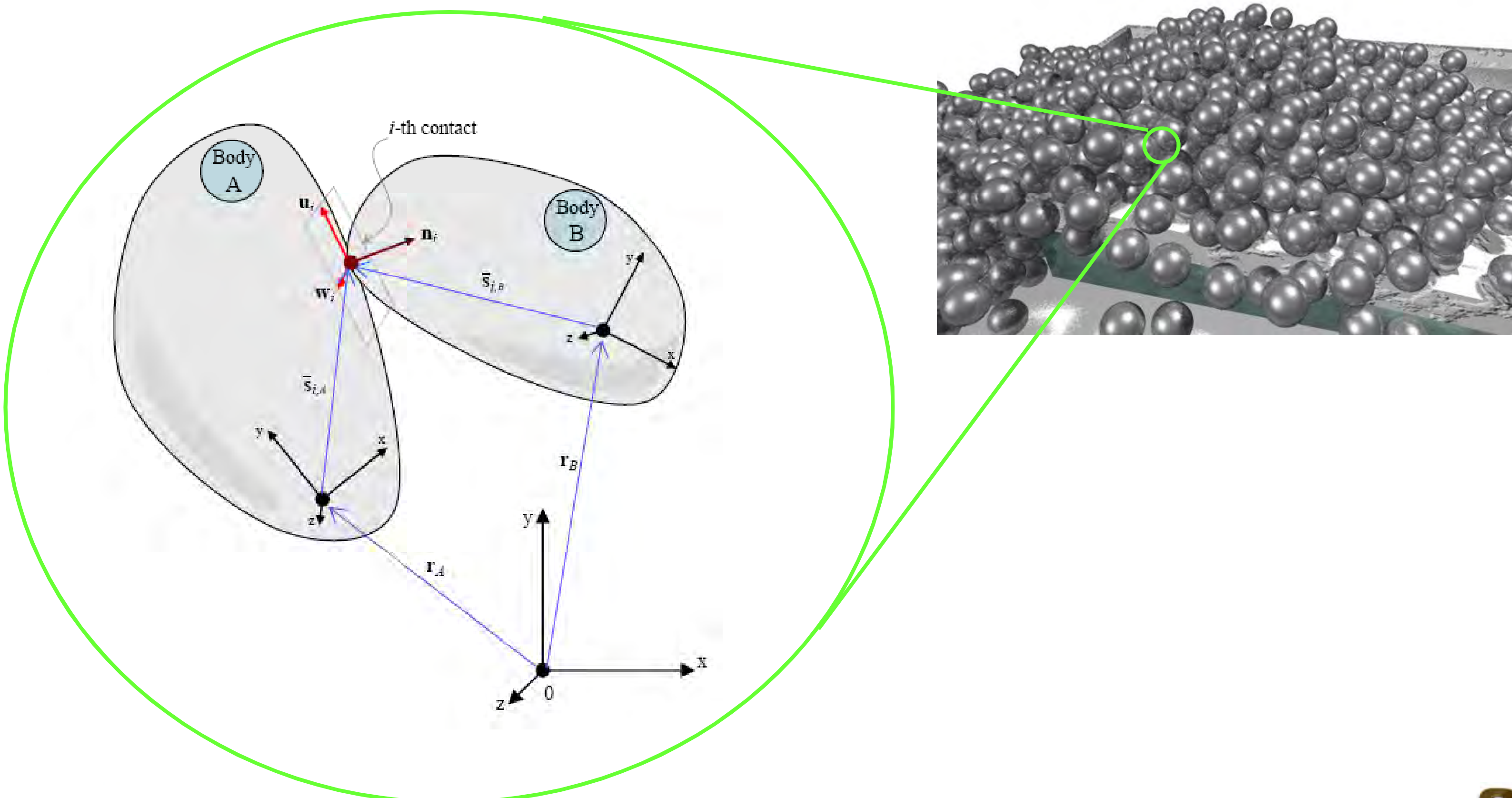
$$\Upsilon^\circ = \left(\bigoplus_{i \in \mathcal{A}(\mathbf{q}^l, \epsilon)} \mathcal{FC}^{i\circ} \right)$$

$\mathcal{FC}^i \in \mathbb{R}^3$ represents friction cone associated with i^{th} contact

CCP assumes following form: Find such that

$$\gamma \in \Upsilon \perp -(\mathbf{N}\gamma + \mathbf{d}) \in \Upsilon^\circ$$

- Numerical solution can leverage parallel computing



CPU vs. GPU – Flop Rate
[GFlop/Sec]

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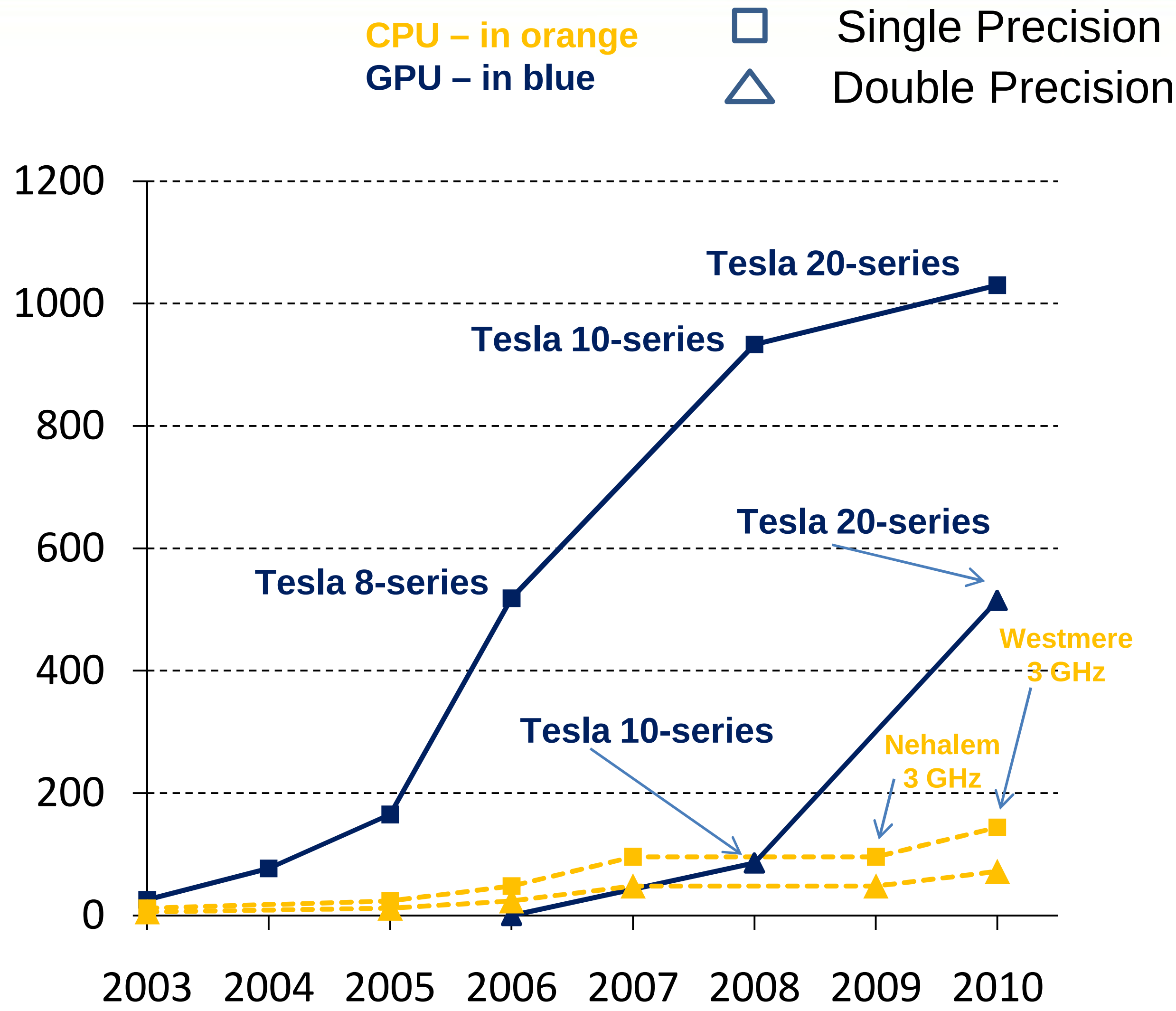
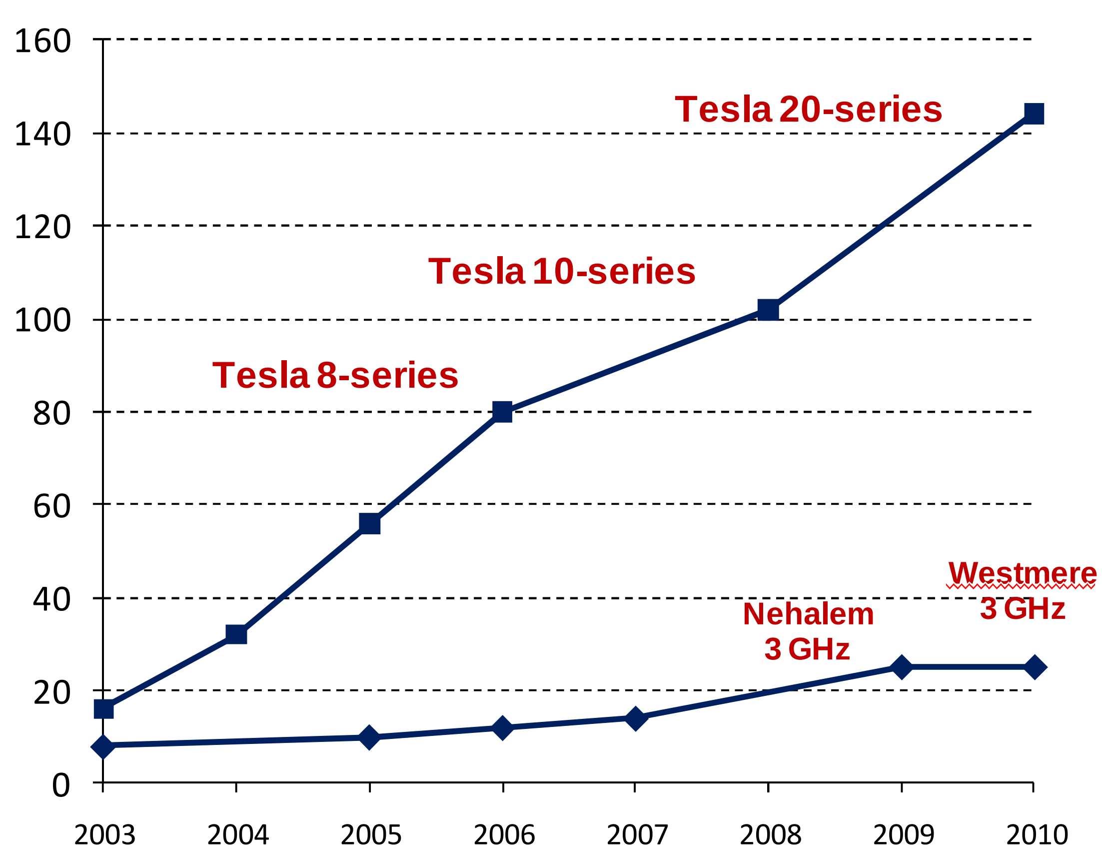
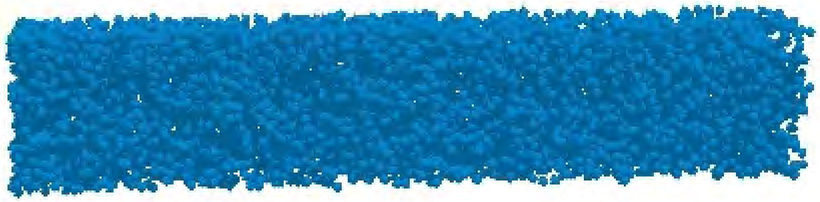


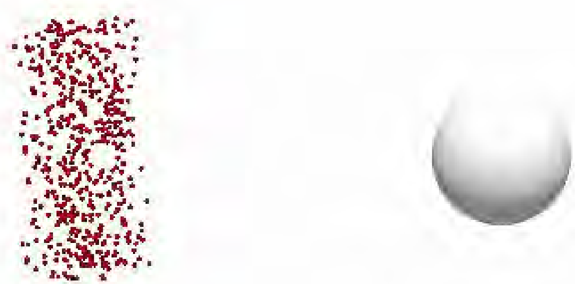
CPU vs. GPU– Memory Bandwidth
[GB/sec]



Mixing 40,000 Spheres on the GPU

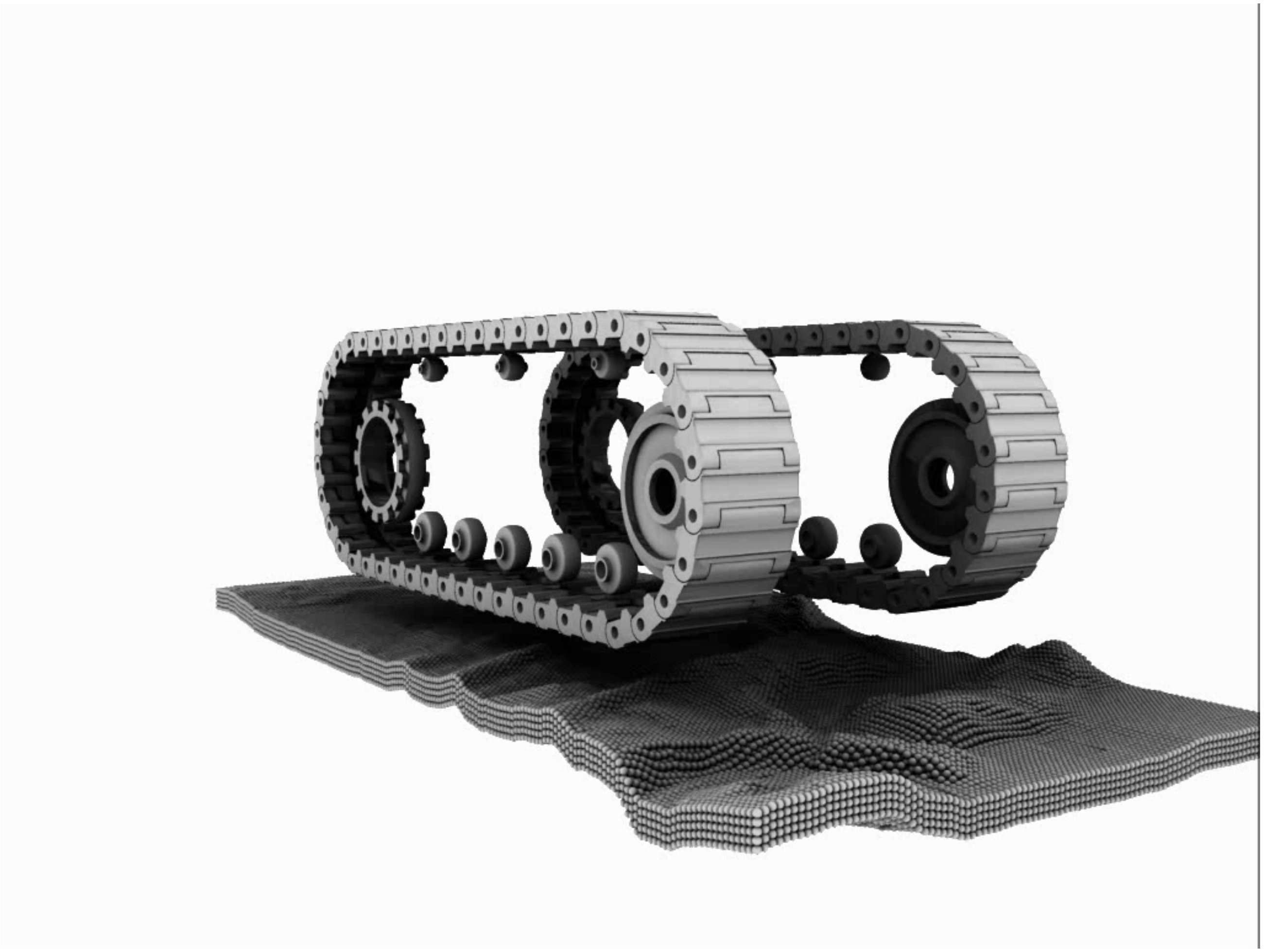


300K Spheres in Tank
[parallel on the GPU]



1.1 Million Rigid Spheres
[parallel on the GPU]

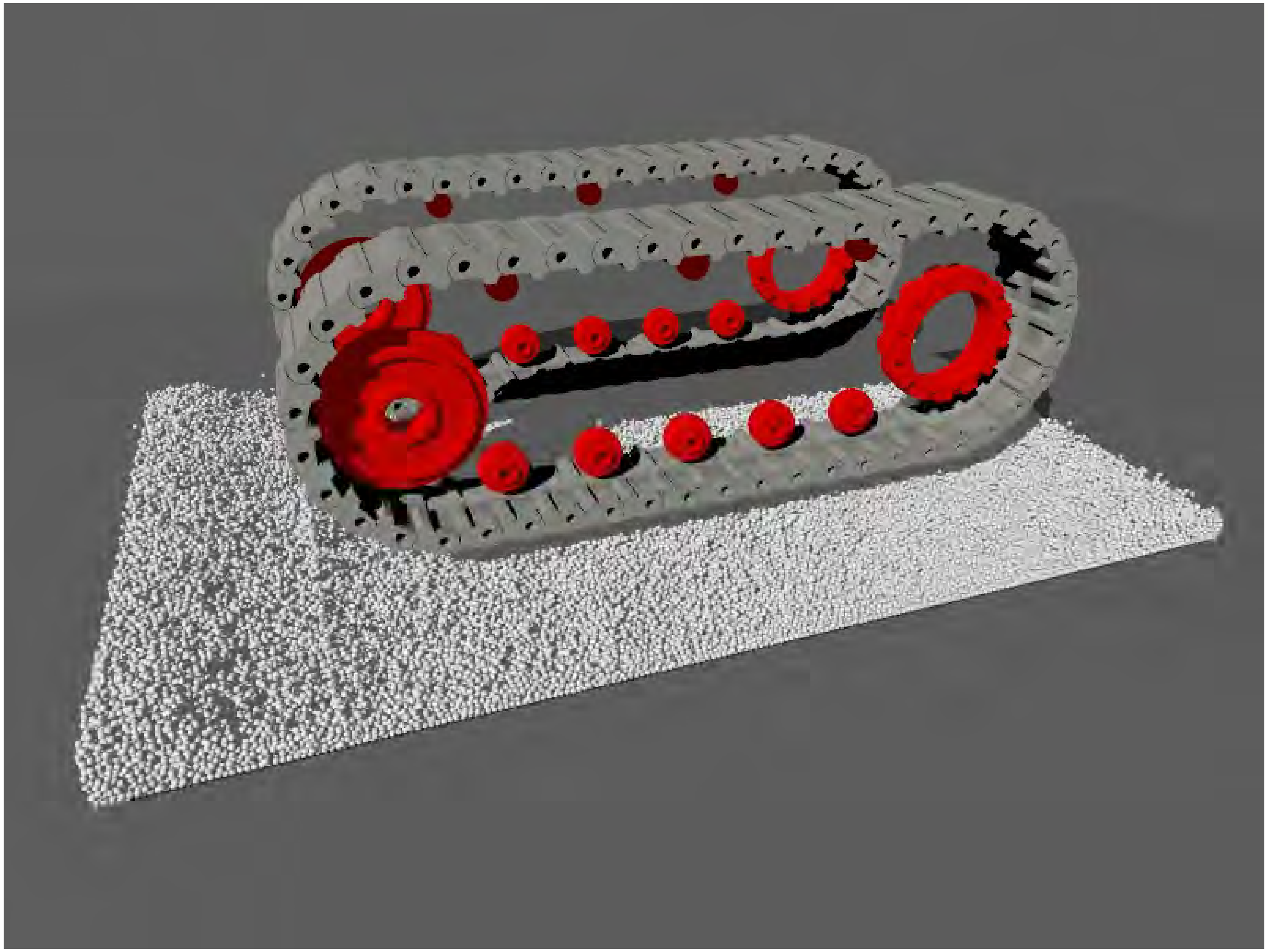
Computational dynamics
Tracked vehicle mobility



Simulation Setup:

- Driving speed: 1.0 rad/sec
- Length: 12 seconds
- Time step: 0.005 sec
- Computation time: 18.5 hours
- Particle radius: .027273 m
- Terrain: 284,715 particles

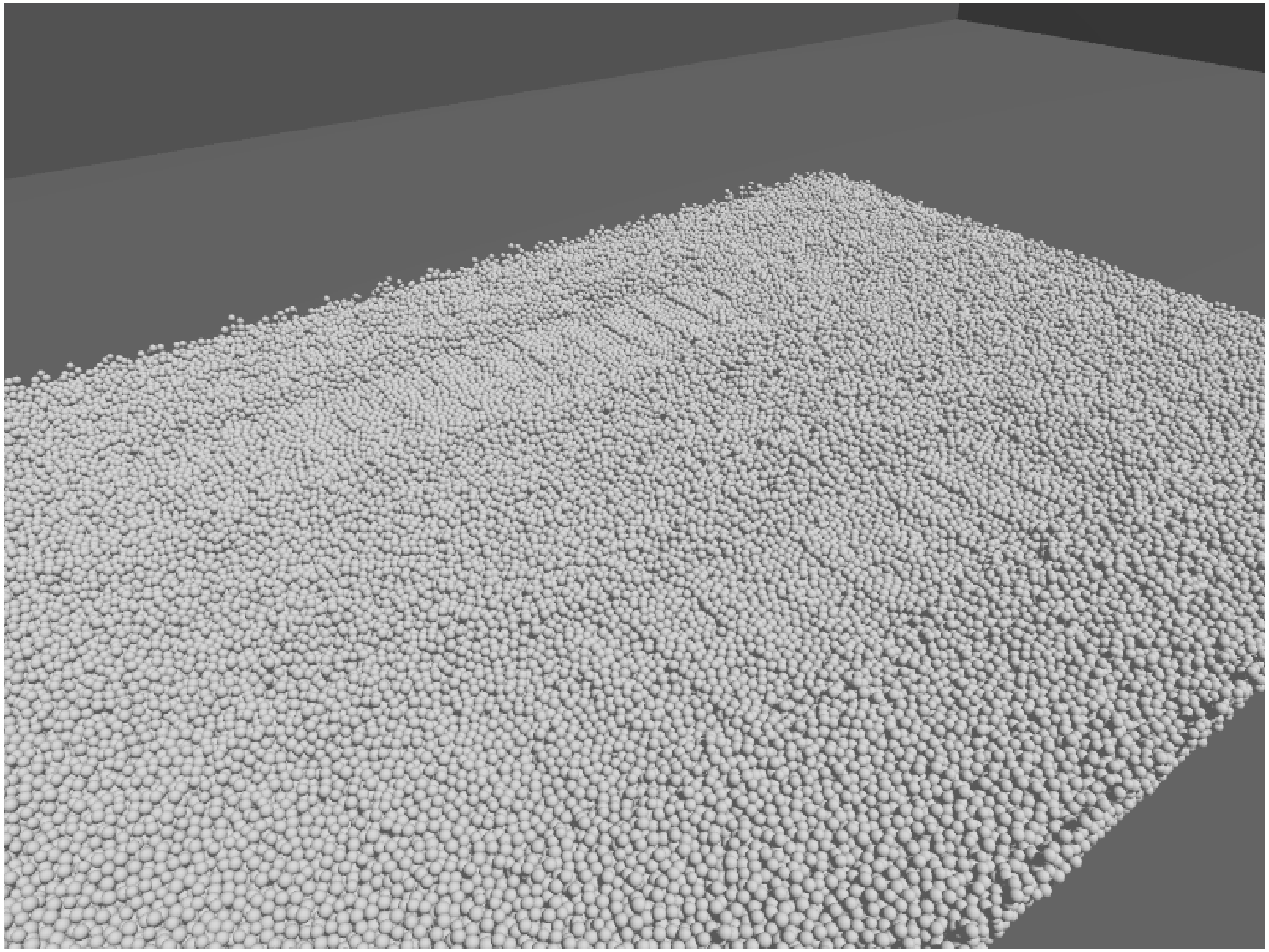
Track Simulation



Parameters:

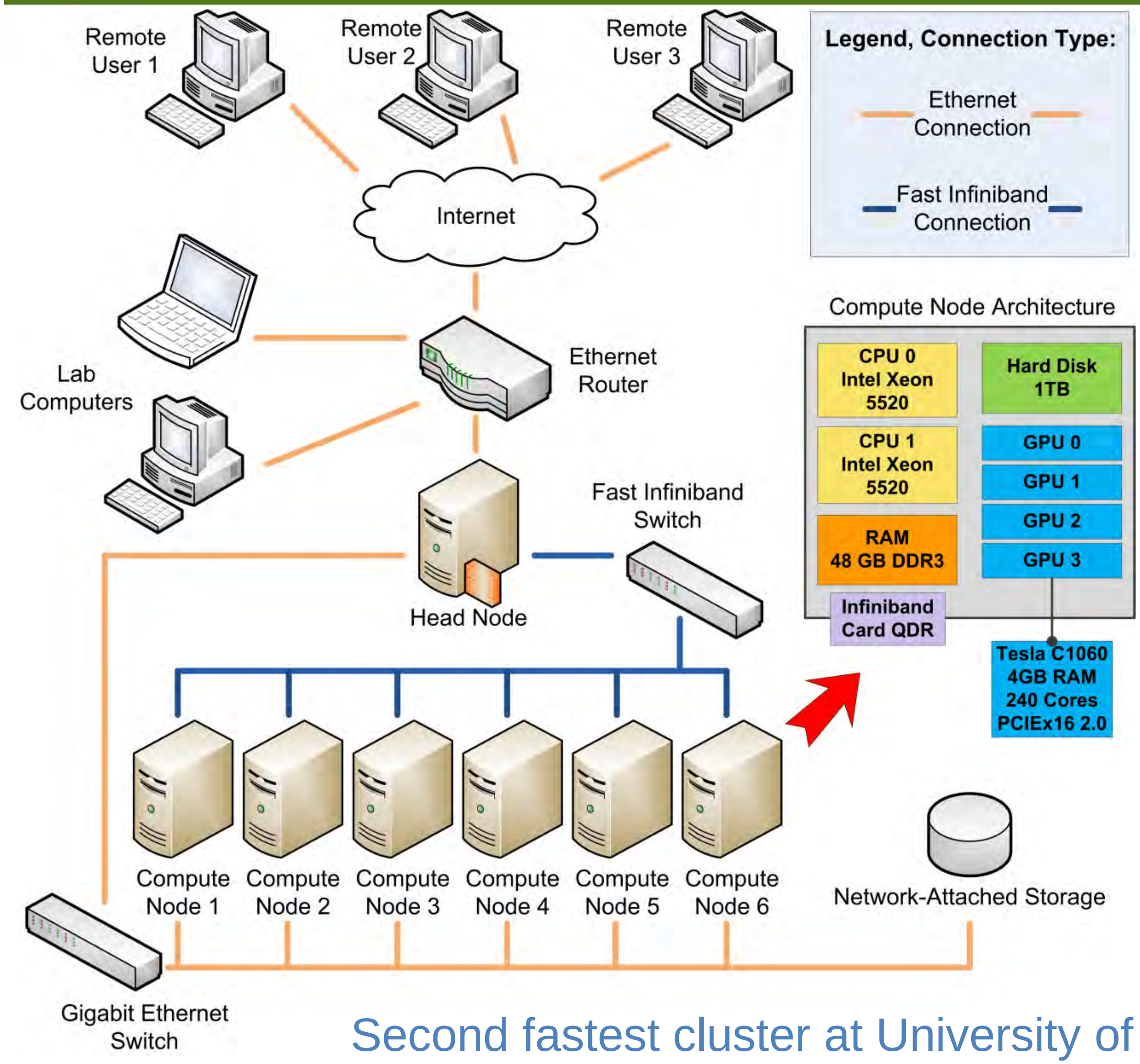
- Driving speed: 1.0 rad/sec
- Length: 10 seconds
- Time step: 0.005 sec
- Computation time: 17.8 hours
- Particle radius: .025±.0025 m
- Terrain: 467,100 particles

Track Footprint



A Heterogeneous Computing Template for Computational Dynamics

Heterogeneous Cluster



Second fastest cluster at University of Wisconsin-Madison

Computation Using Multiple CPUs
[DEM solution]

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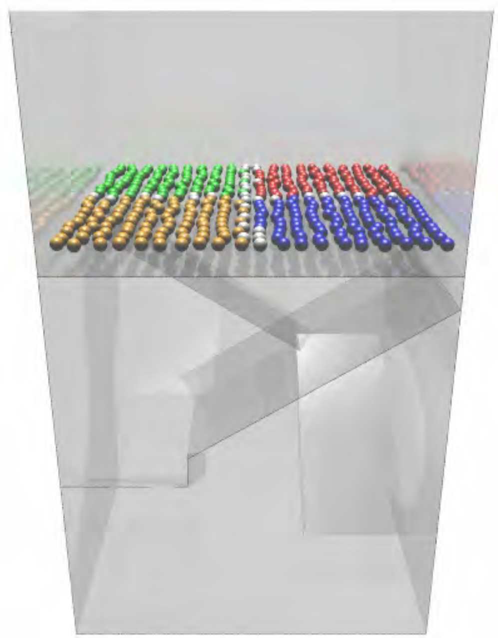
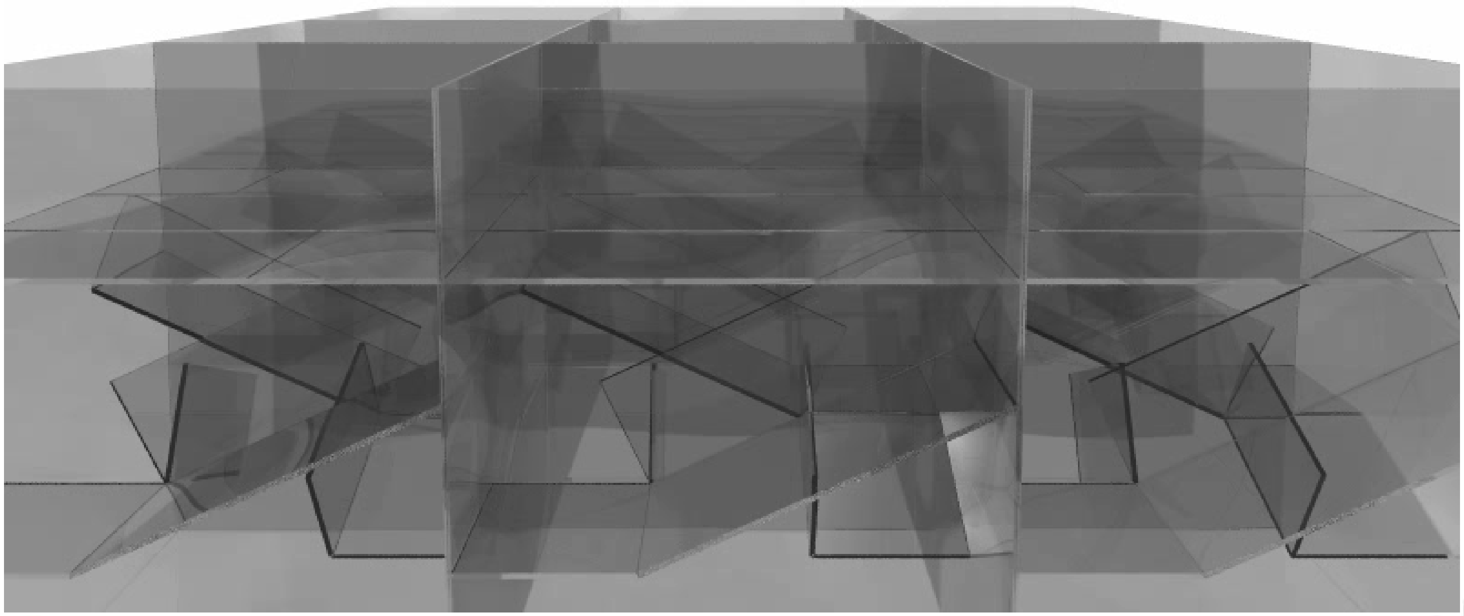
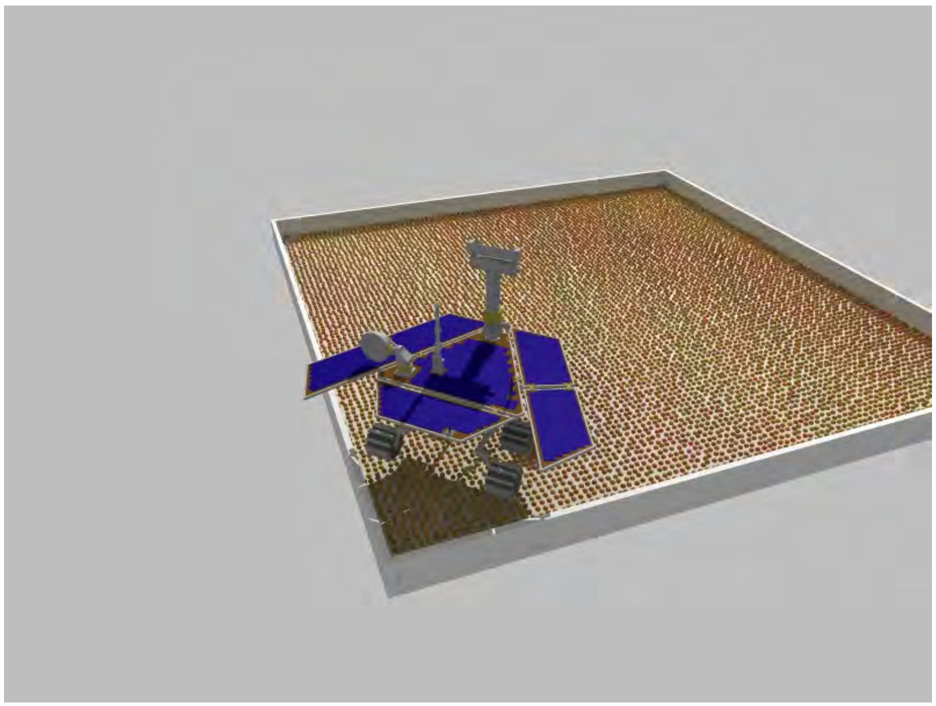
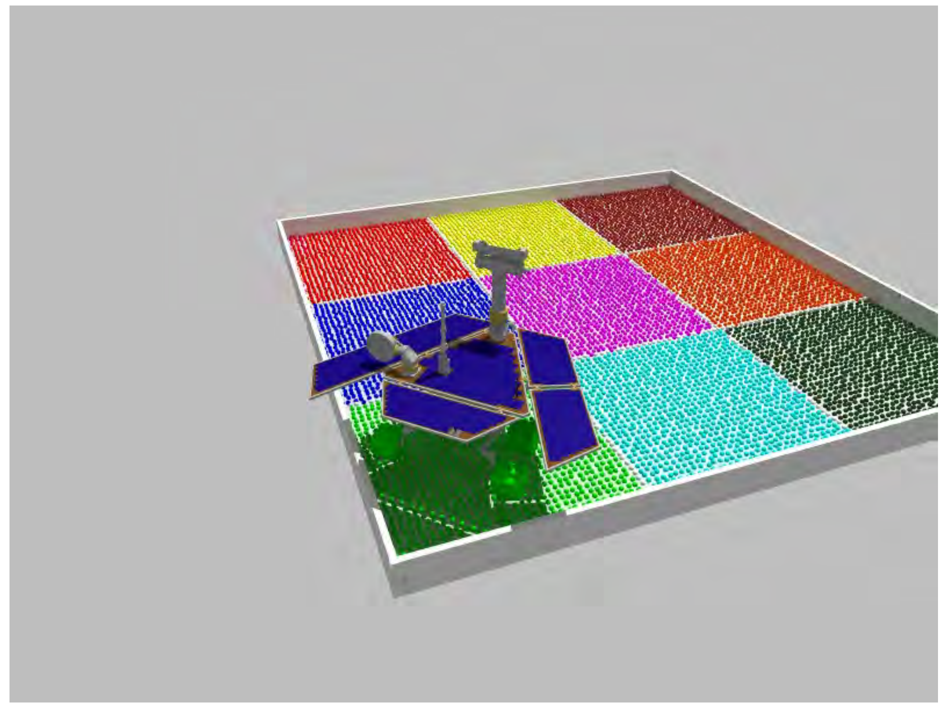


Computation Using Multiple CPUs
[DEM solution]



Computation Using Multiple CPUs
[DEM solution]





Computation Using Multiple CPUs
[DEM solution]

Simulation of MRAP impacted by debris

Heterogeneous Computing Template
Five Major Components

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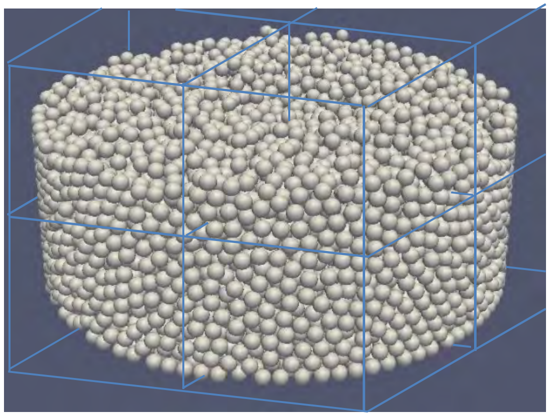
- Computational Dynamics requires
  - Domain decomposition
  - Proximity computation
  - Inter-domain data exchange
  - Numerical algorithm support
  - Post-processing (visualization)



- HCT represents the library support and associated API that capture this five component abstraction

Searching for Better Methods

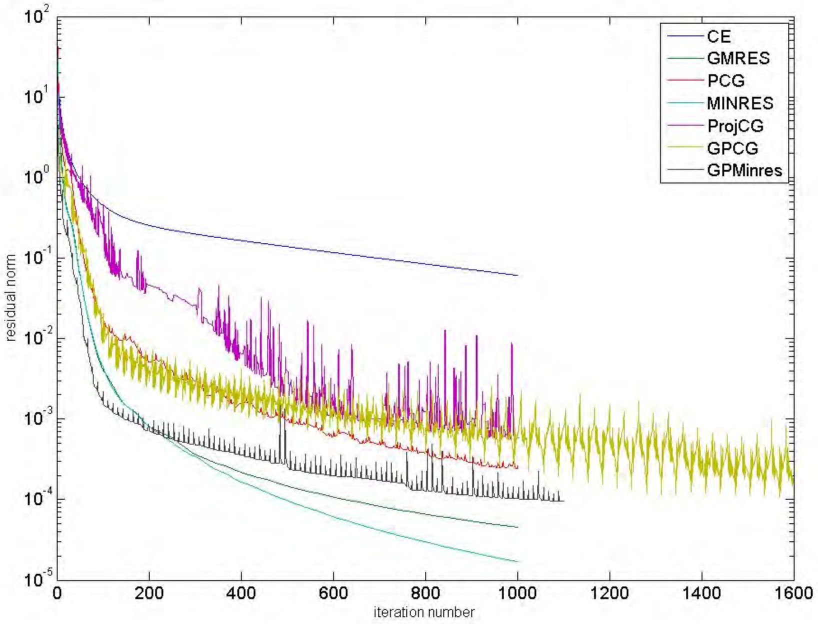
- Frictionless case (bound constraints in place)
  - Gauss-Jacobi (CE)
  - Projected conjugate gradient (ProjCG)
  - Gradient projected conjugate gradient (GPCG)
  - Gradient projected MINRES (GPMINRES)

- Friction case (cone constraints - ongoing)
  - Newton's Method for large bound-constrained problems
    - Uses re-parameterization to handle friction cones (replace with bound constraints)

Numerical Experiments

- Test Problem: 40,000 bodies → 157,520 contacts
- Frictionless

Test Problem (MATLAB)



Method	Iterations	Final Residual Norm	γ_{min}	γ_{max}	Time [sec]
CE	1000	6.11×10^{-2}	0.0	2.0598	1849.5
ProjCG	1002	5.6344×10^{-4}	0.0	2.2286	1235.6
GPCG	1600	1.0675×10^{-4}	0.0	2.6349	382.3644
GPMinres	1100	9.5239×10^{-5}	0.0	2.3090	238.0744
PCG	1000	2.4053×10^{-4}	-1.1116	2.5254	27.9686
GMRES	1000	4.5315×10^{-5}	-1.1635	2.5227	736.3007
MINRES	1000	1.6979×10^{-5}	-1.1316	2.5253	41.5790

Proximity Computation

GPU Collision Detection (CD)

- 30,000 feet perspective:
  - Carry out spatial partitioning of the volume occupied by the bodies
    - Place bodies in bins (cubes, for instance)
  - Follow up by brute force search for all bodies touching each bin
    - Embarrassingly parallel

Example: Ellipsoid-Ellipsoid CD

$$\mathbf{d} = \mathbf{P}_1 - \mathbf{P}_2 = \left(\frac{1}{2\ {}_{1}}\mathbf{M}_1 + \frac{1}{2\ {}_{2}}\mathbf{M}_2\right)\mathbf{c} + (\mathbf{b}_1 - \mathbf{b}_2)$$

$$\frac{\partial \mathbf{d}}{\partial\ {}_i} = \frac{\partial \mathbf{P}_1}{\partial\ {}_i} - \frac{\partial \mathbf{P}_2}{\partial\ {}_i} \quad , \quad \frac{\partial^2 \mathbf{d}}{\partial\ {}_i \partial\ {}_j} = \frac{\partial^2 \mathbf{P}_1}{\partial\ {}_i \partial\ {}_j} - \frac{\partial^2 \mathbf{P}_2}{\partial\ {}_i \partial\ {}_j}$$

$$\boxed{\frac{\partial \mathbf{P}}{\partial\ {}_i} = \left(\frac{1}{2}\mathbf{M} - \frac{1}{8\ {}^{3}}\mathbf{M}\mathbf{c}\mathbf{c}^T\mathbf{M}\right)\frac{\partial \mathbf{c}}{\partial\ {}_i}}$$

$$\boxed{\begin{aligned}\frac{\partial^2 \mathbf{P}}{\partial\ {}_i \partial\ {}_j} &= \left(-\frac{1}{8\ {}^{3}}\mathbf{M} + \frac{3}{32\ {}^{5}}\mathbf{M}\mathbf{c}\mathbf{c}^T\mathbf{M}\right)\mathbf{c}^T\mathbf{M}\frac{\partial \mathbf{c}}{\partial\ {}_j}\frac{\partial \mathbf{c}}{\partial\ {}_i} \\ &\quad - \frac{1}{8\ {}^{3}}\left[(\mathbf{c}^T\mathbf{M}\frac{\partial \mathbf{c}}{\partial\ {}_i})\mathbf{M} + \mathbf{M}\mathbf{c}(\frac{\partial \mathbf{c}}{\partial\ {}_i})^T\mathbf{M}\right]\frac{\partial \mathbf{c}}{\partial\ {}_j} \\ &\quad + \left(\frac{1}{2}\mathbf{M} - \frac{1}{8\ {}^{3}}\mathbf{M}\mathbf{c}\mathbf{c}^T\mathbf{M}\right)\frac{\partial^2 \mathbf{c}}{\partial\ {}_i \partial\ {}_j}\end{aligned}}$$

$$\varepsilon : \frac{x^2}{r_1^2} + \frac{y^2}{r_2^2} + \frac{z^2}{r_3^2} = 1$$

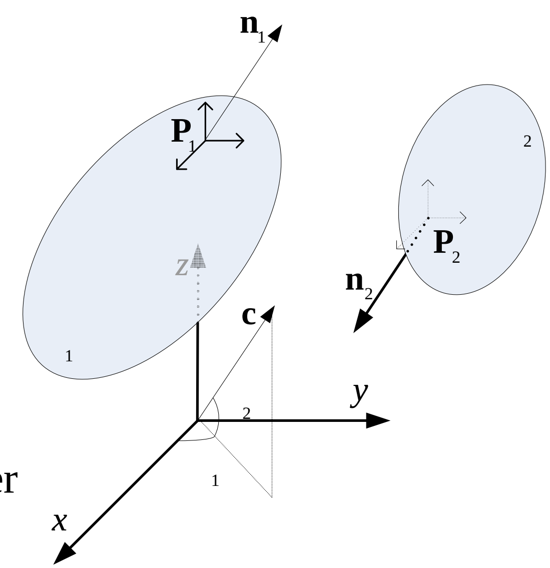
$\mathbf{A}$ **:** Rotation Matrix

$$\mathbf{M} = \mathbf{A}\mathbf{R}^2\mathbf{A}^T$$

$$\mathbf{R} = diag(r_1, r_2, r_3)$$

$\mathbf{b}$ **:** Translation of ellipsoids center

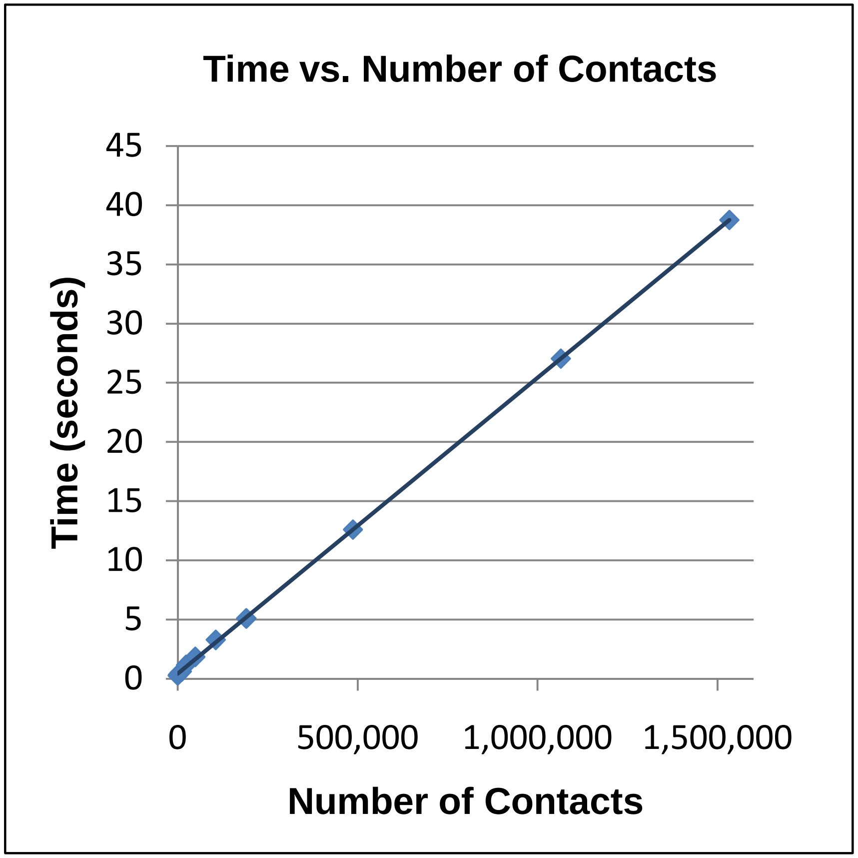
$$^2 = \frac{1}{4}\mathbf{n}^T\mathbf{M}\mathbf{n}$$

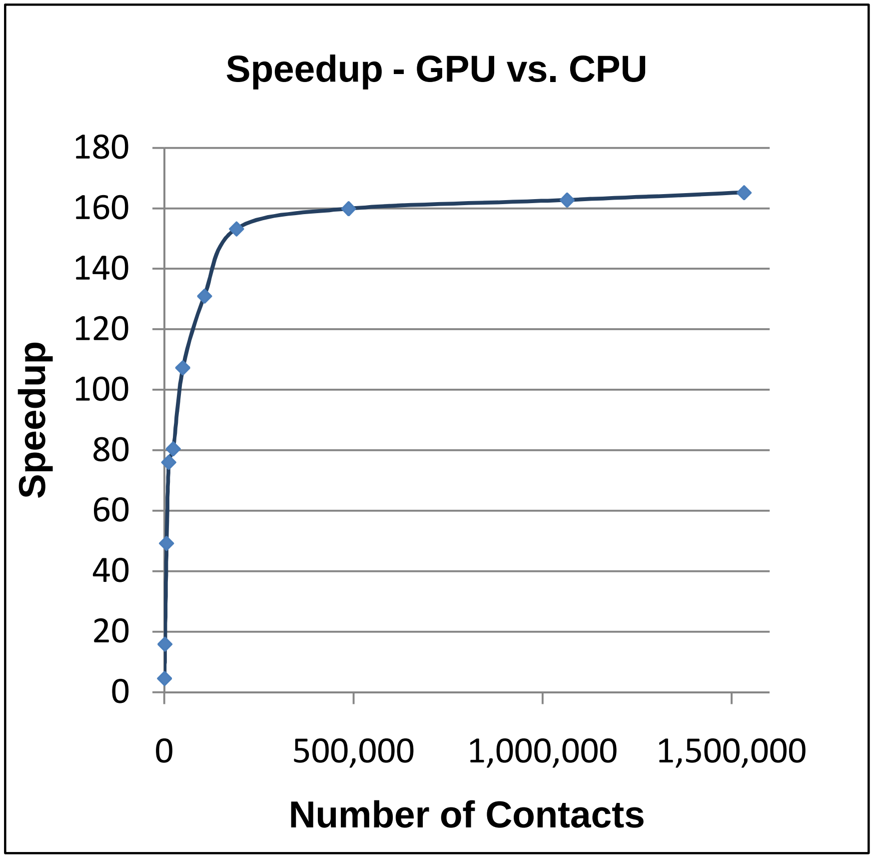


$$\mathbf{d} = \mathbf{P}_1 - \mathbf{P}_2$$

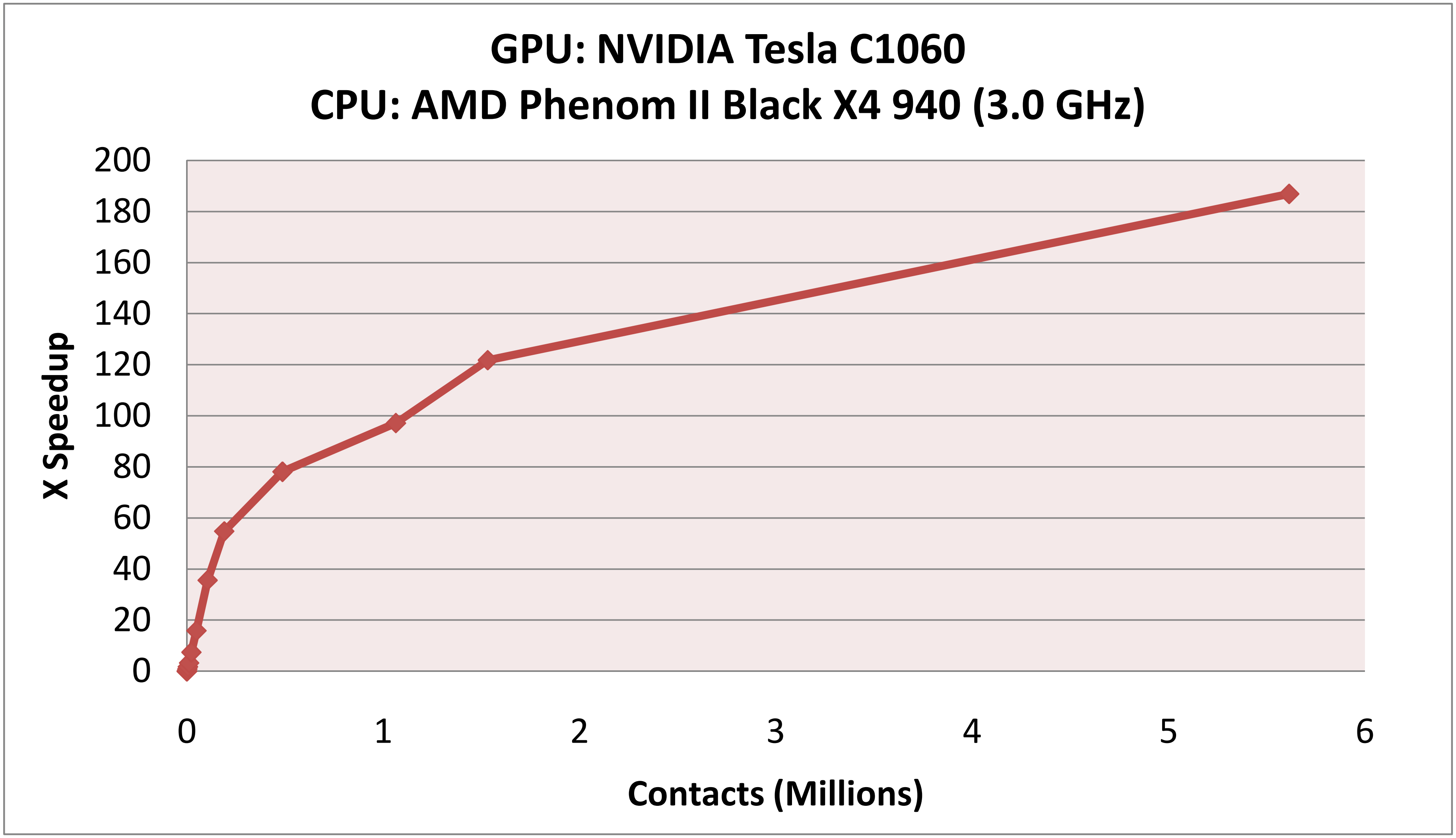
$$\min_{\alpha_1, \alpha_2} \left\| d(\alpha_1, \alpha_2) \right\|^2$$

Ellipsoid-Ellipsoid CD: Results

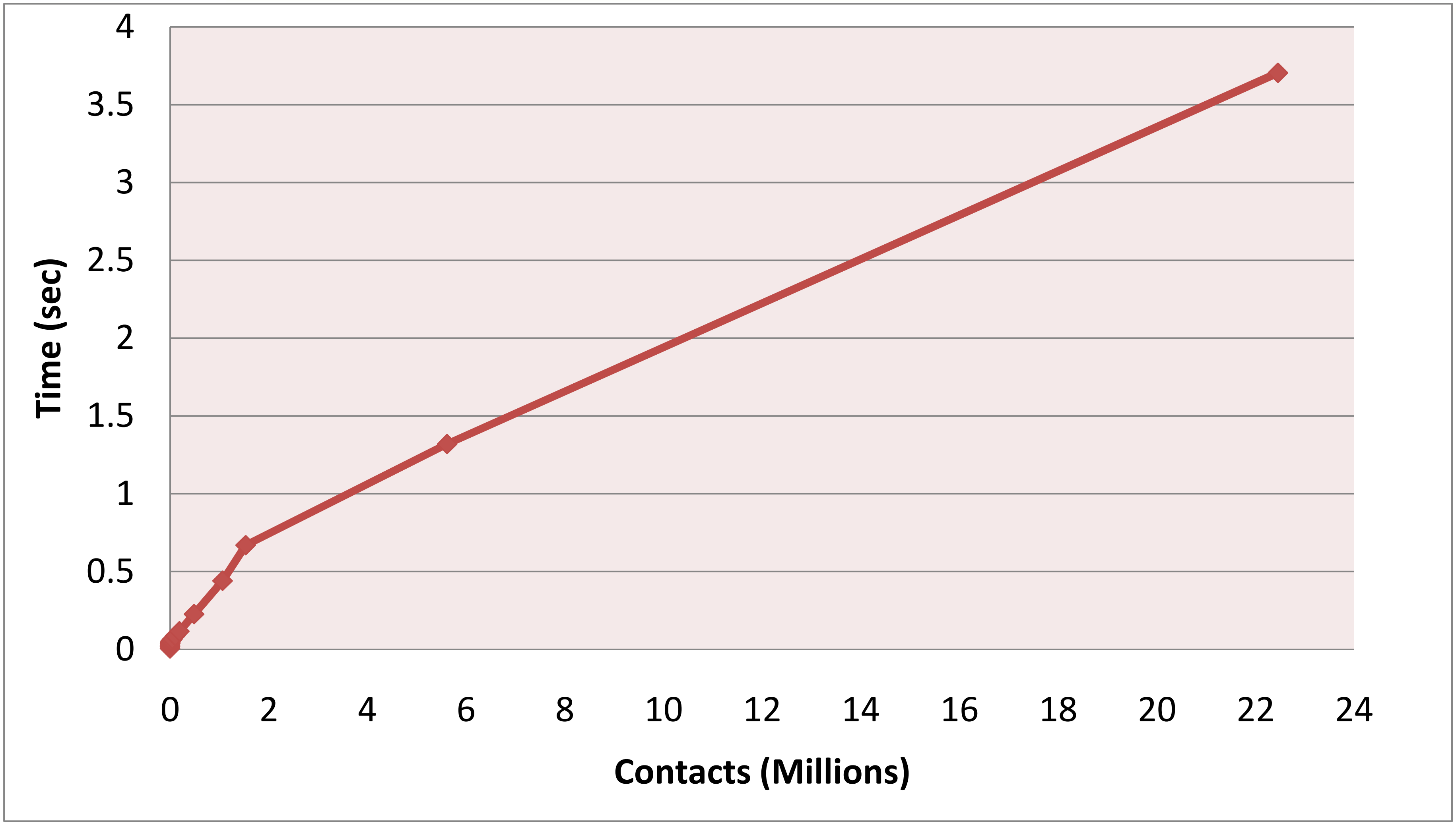




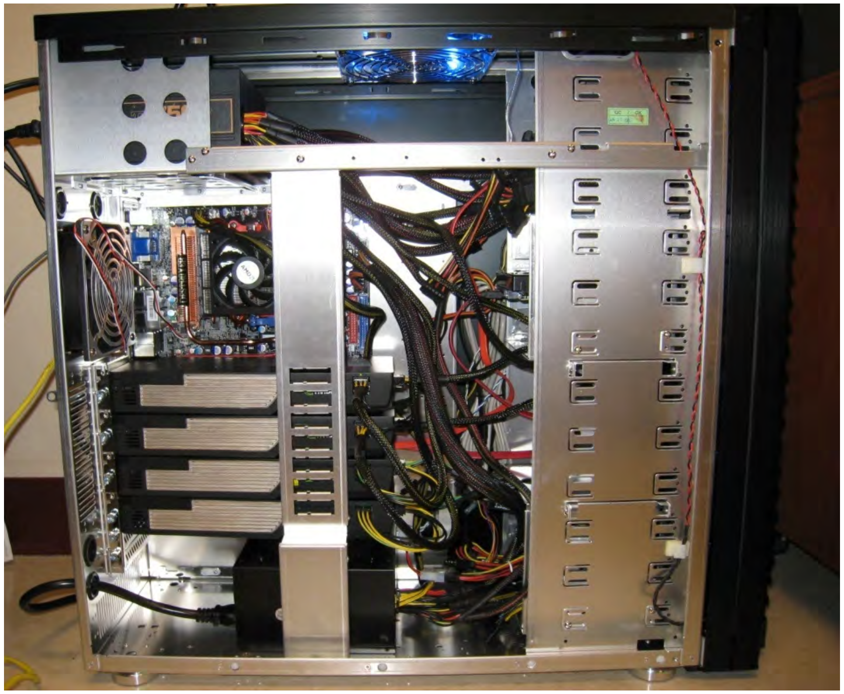
Speedup GPU vs. CPU (sequential Bullet)
[results reported are for spheres]



Parallel Implementation: Number of Contacts vs. Detection Time [results reported are for spheres]



Assembled Quad GPU Machine



Processor: AMD Phenom II X4 940 Black

Memory: 16GB DDR2

Graphics: 4x NVIDIA Tesla C1060

Power supply 1: 1000W

Power supply 2: 750W

SW/HW Setup

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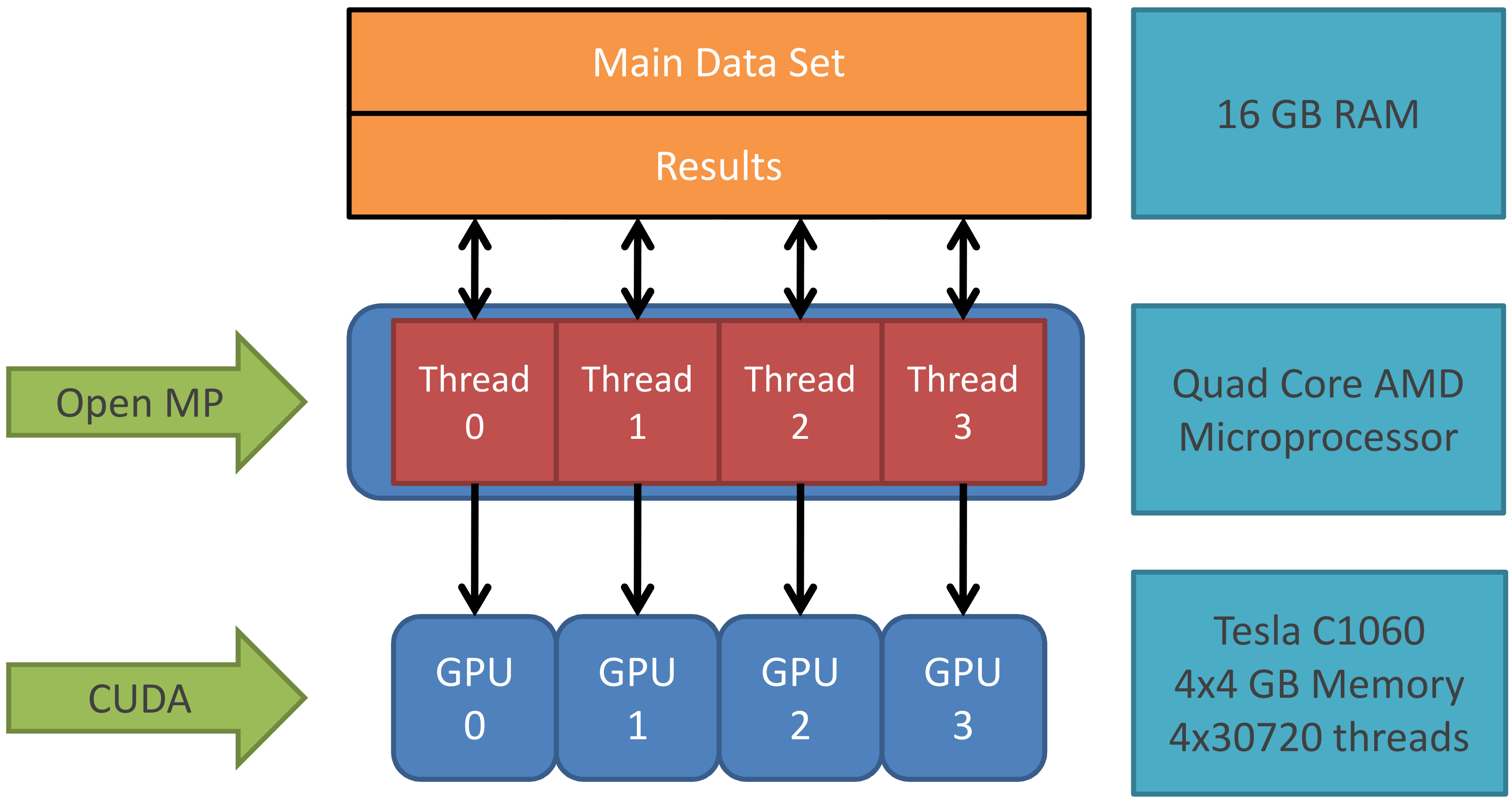
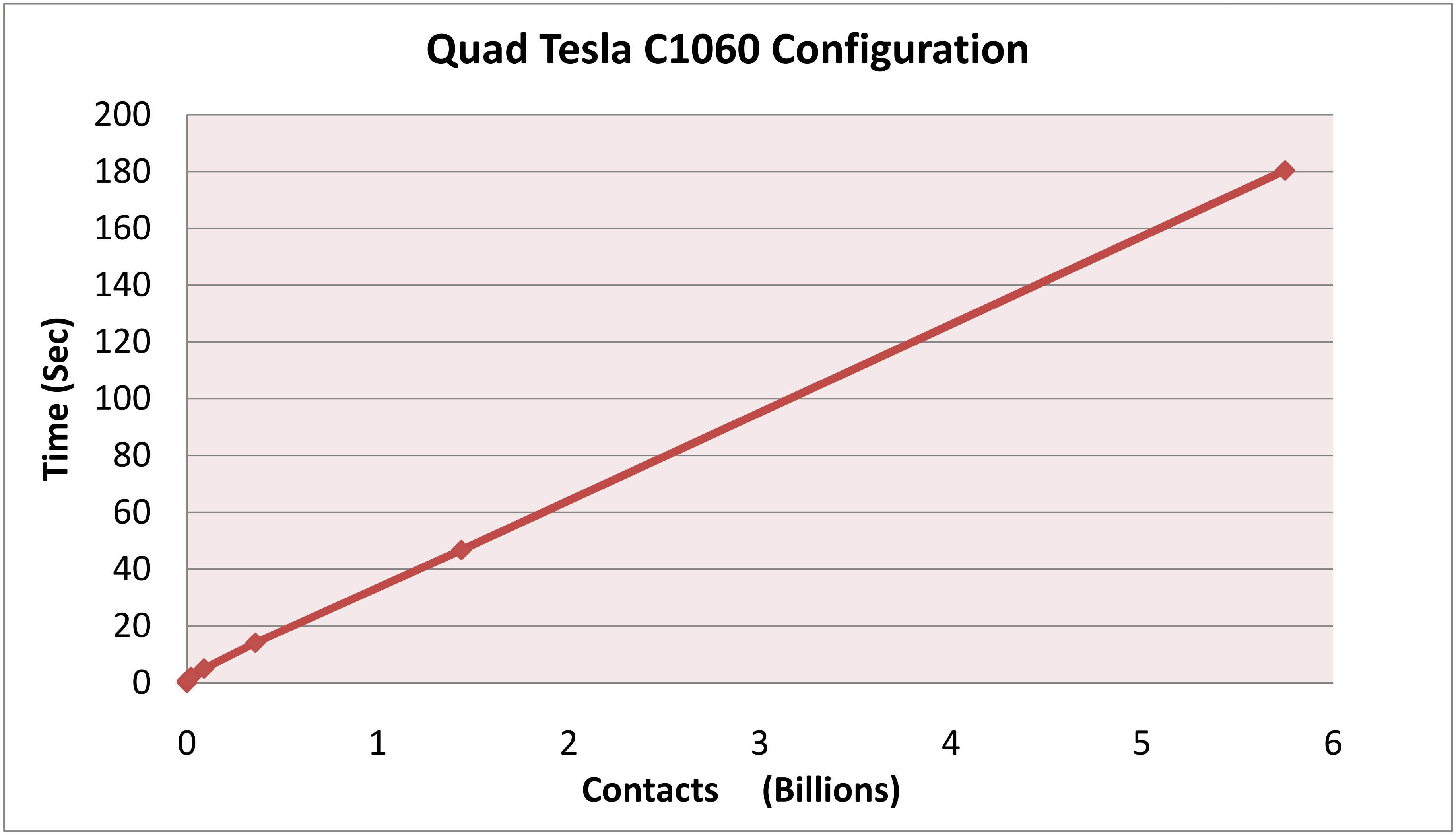


Results – Contacts vs. Time



Conclusions

- HPC will soon enable simulation of billion-body problems
  - Tremendous advances in compute power over the last five years
- Our work: Heterogeneous Computing Template (HCT)
  - HCT draws on symbiosis of CPU + GPU computing
- Accomplishments to date
  - Billion body parallel collision detection
  - Large scale parallel solution of cone complementarity problem
  - Early validation results encouraging

Ongoing/Future Work

- Validation efforts: at CAT, US Army, and JPL
- Massively parallel linear algebra for solution of CCP problem
  - Preconditioned gradient projected Krylov method
- Parallel collision detection for complex geometries
- Multiphysics:
  - Fluid-solid interaction
  - Cohesion
  - Electrostatics

Thank You.